FWP Title: Structure and Phase Transformation of Nanophases… **Name of the Laboratory: LBNL**
FWP Number: KC11A **B&R Code: KC020101**

Program Abstract:

This program aims to understand the fundamental features that underlie the behavior of nanoscale phases embedded in a solid matrix and their role in the evolution of microstructure in materials. Because of the scale and nature of such microstructures, electron microscopy is an integral part of these investigations - as an analytical tool as well as a subject of technique development. The goal is to understand and ultimately gain control of the structure, distribution and shape of nanophase inclusions by establishing the basic relationship between crystallographic variables and microstructural features. Such relationships are put to use both analytically, to examine the structure of particles and defects, and synthetically, to produce new and unique microstructures with defect configurations reflecting composite symmetries. The long-term objective is to develop an understanding of nanoscale inclusions as a function of their size, shape and embedding parameters such as elastic strain and crystallographic alignment. The fundamental principles established using model alloy systems are employed in the design and testing of new materials such as Al-based alloys of interest for energy-related technologies.

Program Impact:

This work has led to an improved understanding of the key role played by embedding parameters in the evolution of microstructures. In particular, the role of crystallographic alignment and confinement in a solid matrix on the behavior of nanoscale particles has been elucidated and utilized in thin film growth and precipitation reactions. This program generates fundamental knowledge necessary to understand how nanomaterials interact with a solid environment, thus providing important information for energy-related engineering applications of nanomaterials in the real world. The combination of advanced electron microscopy instrumentation and techniques available at NCEM with expertise in computer modeling and materials synthesis goes beyond the abilities of a single investigator program.

FY 2009 Authorized Budget (New BA): $250k

Program Personnel Supported in FY2009:

Principal Investigators: U. Dahmen 5%, V. Radmilovic 50%
Postdoctorals: A. Gautam 40%, M. Rossell-Abrodos 10%

Interactions:

University of Alberta (D. Mitlin)
UC Davis (M. Asta)
Sandia National Laboratory (J. Hamilton)
Oxford University (E. Marquis)
RPI (D. Lewis)

FWP Title: Soft Matter Electron Microscopy **Name of the Laboratory: LBNL**
FWP Number: KC11BN **B&R Code: KC020101**

Program Abstract:
Our objective is to determine the underpinnings of ion transport in polymer membranes. We focus on self-assembled nanostructures formed by bio-inspired peptoids and synthetic block copolymers within which transport is restricted to one of the nanostructures. Our objective is to determine the geometry and chain configurations that lead to the most efficient solid-phase ion-transporting channel. Spatially resolved electron microscopy and energy-loss spectroscopy are crucial for obtaining the relationship between morphology and transport. The proposed microscopy techniques focus on maximizing spatial and energy resolution while minimizing radiation exposure and damage. This will be achieved by using novel techniques to manipulate and detect the incident, transmitted, and scattered electrons. In addition, we will use aberration-correctors, high brightness instruments, and novel 3D image reconstruction algorithms. *In-situ* electron microscopy experiments for investigating the dynamic nature of soft materials on molecular and sub-molecular length scales have been designed. We will develop materials with unique properties such as membranes that become wetter when they are heated in air and mechanically robust solid electrolytes for battery applications.

Program Impact:
This is a unique program with PIs drawn from three different areas: soft matter synthesis (Balsara and Zuckermann), electron microscopy of biological samples (Downing and Glaeser), and high resolution and in-situ electron microscopy of hard matter (Kisielowski and Minor). The projects that are being pursued lie at the intersection of these areas. The issue that binds the projects together is the need for high resolution imaging of the ion-conducting channels in the materials. Our lack of fundamental understanding of the factors that control ion transport in synthetic nanostructures prevents the widespread use of batteries and fuel cells for transportation, grid balancing, and other energy-related devices.

FY 2009 Authorized Budget (New BA): $750K

Program Personnel Supported in FY2009:
Principal Investigators: N. Balsara 5%, A. Minor 10%, K. Downing 5%
Technical Staff: B. Pesavento 70%
Postdoctorals: F. Allen 100%, D. Alloyeau 100%, S. Yakovlen 70%, M. Park 40%, H. Guo 10%, X. Wang 20%
Graduate Students: H. Huang 50%, K. Beers 30%, G. Stone: 30%, S. Patel 10%

Interactions:
Collaborations established with A. Jackson on neutron scattering at NIST, Gaithersburg, MD, M. Banaszak on theory of self-assembly of ion-containing block copolymers at A. Mickiewicz University, Poland, and J. Batenburg on discrete tomography at the University of Antwerp, Belgium.

FWP Title: Mechanical Behavior of Advanced Materials **Name of the Laboratory: LBNL**
FWP Number: KC13 **B&R Code: KC020102**

Program Abstract:

This program is focused on the development of an understanding of the mechanical behavior of next generation structural materials, in particular involving mechanical properties that are influenced by factors operating at a wide range of length-scales. Our goal is to design, synthesize, and characterize (structurally and mechanically) a new series of hybrid structural materials, whose unique properties derive from hierarchical architectures controlled over length-scales from nano to macro dimensions. The inspiration for these structures is biological; our goal is to defeat the "law of mixtures" (as in Nature) by devising complex hierarchical structures comprising weak constituents into strong and tough (*non-biological*) hybrid (polymer-ceramic & metal-ceramic) materials, which display far superior properties to their individual constituents. The research approach combines mechanistic understanding of structural behavior at multiple length-scales, the ability to synthesize such materials using novel techniques, the control of structural features (particularly interfaces) at the nanoscale, the ability to mechanically and structurally characterize such structures at atomic, molecular, nano, micro to macroscopic dimensions, and the evaluation of the suitability of these structures/systems for technological (energy-related) applications.

Program Impact:

This is a program that combines the talents of processing and mechanical/structural characterization resident in the research groups of the two PIs in order to develop new lightweight structural materials that are intended for potential applications in energy-related technologies such as energy generation (power-turbines), energy transmission (pipelines) and transportation (automobiles). It harnesses the unique facilities at LBNL of the Advanced Light Source (for computed tomography) and the National Center for Electron Microscopy (for high-resolution structural characterization). We believe that our initial efforts to create (for the first time) a bulk structural material that mimics the hierarchical structure of biological materials, in this case nacre and bone, has been remarkably successful in that using "routine materials", *i.e.*, alumina, PMMA and sugar and salt dopants, we have processed one of the toughest ceramic materials ever made. If we can be successful in generating similar microstructures using high melting point metals instead of polymers as the "lubricant phase", we believe that we will have developed a family of lightweight, high-temperature materials with both strength and toughness at ambient and elevated temperatures, which could have a major impact in the energy-related applications noted above.

FY 2009 Authorized Budget (New BA): $700k

Program Personnel Supported in FY2009:

Principal Investigators: R. Ritchie 5%, A. Tomsia 30%
Postdoctorals: D. Alsem 100%, K. Koester 10%, M. Launey 100%
Graduate Students: S. Martin 40%, E. Zimmermann 50%

Interactions:

Oak Ridge National Laboratory (high toughness ceramics); Lawrence Livermore National Laboratory (bicrystal fabrication, embedded nanoarrays); Argonne National Laboratory (*in situ* stress measurements); National Institute of Standards and Technology, (wetting); National Center for Electron Microscopy, LBNL (high-resolution imaging); Advanced Light Source, LBNL (residual stress measurement); Sandia National Laboratory (wetting, liquid/solid interfaces); Idaho Engineering National Laboratory (adhesion); Los Alamos National Laboratory (fundamentals of interfacial and layered structures); Cal Tech (toughness, glassy metals); MIT (interfacial segregation); Max-Planck Institute, Stuttgart (fundamentals of dissimilar interfaces); University of Karlsrule (freeze-casting); Imperial College, London (processing, microscopy); University of Mons, Belgium (molecular dynamics calculations).

FWP Title: Electronic Materials **Name of the Laboratory: LBNL**
FWP Number: KC1201 **B&R Code: KC020103**

Program Abstract:
The Electronic Materials Program advances the fundamental understanding of the materials science of semiconductors. The research focuses on the relationships between synthesis and processing conditions and the structure, properties, and stability of semiconductor materials systems. Progress in these areas is essential for the performance and reliability for technologies that lie at the heart of the DOE mission including ultrahigh efficiency photovoltaic energy conversion devices, high efficiency solid-state sources of visible light, visual displays, and of a large variety of sensors and power control systems for energy generation, conservation, distribution and use.

Program Impact:
Under sustained BES funding, the Electronic Materials Program has discovered new classes of semiconducting materials (in particular those based on alloying with "mismatched" elements) and has contributed significantly to the synthesis and fundamental understanding of a large number of elemental and compound semiconductors. Basic research in the Program concerning the interplay of extended defects, compositional fluctuations, and the resulting strain distributions and the light emission mechanism in GaN and InGaN aided the development of solid-state lighting based on this materials system. Program research has established that both In-rich InN and certain II-VI and III-V "highly mismatched alloys" (HMAs) show promise as entirely new types of high efficiency solar cells and other opto-electronic devices. Most recently, isotopically enriched silicon with high chemical purity was used to demonstrate long-lived quantum information storage.
The Electronic Materials Program is a collaborative effort encompassing growth and synthesis of high quality semiconductors in bulk, thin film and nanocrystalline form and studies of their basic electronic, optical, magnetic, and structural properties combined with theoretical modeling. This approach has led to major breakthroughs in semiconductor science.

- Pioneered scientific applications of isotopically controlled semiconductors; performed definitive impurity and self diffusion studies in Group IV and III-V semiconductors using stable enriched isotope superlattices.
- Developed new theory (band anticrossing model) to explain properties of "highly mismatched" alloys (HMAs) such as GaN_1As_{1-x} and discovered new II-VI-based HMAs, including the first multiband semiconductor.
- Contributed significantly to the understanding of InN as a narrow gap semiconductor and established p–type doping across the entire InGaN composition range.
- Pioneered the use of pulsed laser melting for the synthesis of highly non-equilibrium alloys, including HMAs and "spintronic" materials.
- Established fundamental relationship between native defects and the achievable limits for doping.
- Identified Mn interstitials as the crucial defects in ferromagnetic $Ga_{1-x}Mn_xAs$ and established that these defects lead to a thermodynamic limit of the Curie temperature in this alloy system.
- Developed advanced electron microscopy methods to quantify the growth mechanisms of extended defects and to determine the atomistic core structure of dislocations in group III nitride thin films and heterostructures.
- Developed new theory of nucleation of melting/freezing phase transitions for embedded nanocrystals and verified predictions experimentally.

FY 2009 Authorized Budget (New BA): $1,451K

Program Personnel Supported in FY2009:
Principal Investigators: W. Walukiewicz 40%, J. W. Ager III 40%, D. Chrzan 20%, O. D. Dubón, Jr 10%, Z. Liliental-Weber 80%, K. M. Yu 40%
Post-docs: M. Hawkridge 20%, J. Beeman 5%
Graduate Students: C. Boswell 30%, R. Broesler 50%, G. Buchowicz 5%, J. Guzman 20%, M. Jhon 20%, D. Speaks 10%, C.W. Yuan 40%,
Undergraduate Students: K. Cho 10%, H. Smith 20%
Technical Staff: M. Kao 10%

Interactions Internal—National Center for Electron Microscopy, Advanced Light Source, Molecular Foundry. External— Stanford Synchrotron Radiation Center, Cornell, Purdue, Simon Fraser, Princeton, Münster Univ., Germany, LANL, Georgia Tech, MPI Stuttgart, High Pressure Research Center "Unipress" – Polish Academy of Sciences, Ritsumeikan University, Chiba University, UC Santa Barbara

FWP Title: Nanomechanics at Hard/Soft Interfaces **Name of the Laboratory: LBNL**
FWP Number: KC1202 **B&R Code: KC020103**

Program Abstract:

The overall program goal is to advance the fundamental understanding of complex phenomena at the interface of soft and hard nanomaterials. The research focuses on two areas: (i) understanding of transport of liquids, ions, and molecules in nanofluidic channels; (ii) exploring and understanding the nanowire-living cell interfaces for guided cell differentiation. The first area explores the science and engineering of molecular and ionic transport in confined or low-dimensional liquids. Progress in this area will lay the foundations of integrated nanofluidic circuits for manipulating single molecules, as well as new approaches for energy-efficient separations of liquid mixtures. The second area will explore the science at nanostructure-cell interfaces and develop ways to direct harvest electricity from microorganisms. Microorganisms can be harnessed through fuel cells to convert organic wastes into electricity. In a typical microbial fuel cell (MFC), microbes act as living catalysts to convert organic materials into electricity. However, MFCs are not yet viable for most applications due to a lack of understanding of underlying electron harvesting mechanism and a low efficiency. Nanowire arrays will be utilized as a powerful tool to understand electron flow in complex microbial systems, and harvest electricity in a nanowire-based microbial fuel cell (NW-MFC).

Program Impact:

Confinement of electrons, photons, and phonons in nanostructured solid materials produces complex phenomena due to the interplay between the size of solid materials and a critical length scale, such as wavelength and mean free path, associated with these fundamental particles. Research on this has received wide attention over the last four decades. In contrast, confinement of liquids and liquid-based molecular transport, although equally interesting and complex, has received relatively less inquiry. It is clear that the range of length scales over which various intermolecular forces operate in aqueous solutions fall within the range of 1-100nm. Hence, if aqueous solutions were confined to these length scales, we would be able to observe transitions in their behavior and, subsequently, we would be able to identify and realize strategies to manipulate their properties for important engineering applications such as sensing, ion-selective transport, and electrochemical energy storage.

In addition, nanowire arrays can be directly interfaced with living cells including diverse microbes, which enables us to understand and control the nanowire/living cell interface. With a precise control of nanowires/microbes interface, nanowire-based microbial fuel cell (NW-MFC) can be developed to probe electron transfer process at microbes/electrode interface, and ultimately harvest electrical energy in a highly efficient manner.

FY 2009 Authorized Budget (New BA): $230k

Program Personnel Supported in FY2009:

Postdoctorals: J. Tang 80%, D. Xu 80%
Graduate Students: D. Coso 60%, C. Duan 30%, J. Feser 60%, S. Yee 20%

Interactions:

Other BES-MSED programs: Chemical and Mechanical properties of Surfaces, Interfaces and Nanostructures (FWP No. KC3101, Organic-inorganic Nanocomposites (KC3104), Nanostructured thermoelectrical materials (KC 1205) and Nanowire-based functional assemblies (KC 1204) – none have direct overlap.

External collaboration with Prof. H. Daguchi at University of Tokyo for theoretical simulation.

FWP Title: Characterization of Functional Nanomachines **Name of the Laboratory: LBNL**
FWP Number: KC1203 **B&R Code: KC020103**

Program Abstract:

This project establishes a multi-disciplinary team at LBNL with the goal of developing, characterizing, and better understanding the fundamental behavior of mechanical devices at the nanoscale. Two paths are followed toward this goal. First, naturally occurring bio-motors are harnessed to take advantage of the molecular mechanisms provided by Nature. Second, new synthetic molecular machines are purposefully designed in a molecule-by-molecule fashion. The program should yield two new categories of mechanically functional nano-assemblies. The first involves chemically engineered molecules, purposefully designed with specific mechanical functions in mind. The second involves exploitation of the unique properties of carbon nanotubes to create novel, nanomechanical devices. A common theme that runs throughout this program is to explore the mechanical response of a nanomaterial or a nanodevice in response to an external force (such as pressure or electromagnetic stimulus) or internal changes (such as phase transitions and chemical reactions), and to clarify the mechanisms by which it converts energy from one form to another. These efforts will help to form the scientific basis underlying new molecular-mechanical nanotechnology with applications in areas of importance to DOE. Such areas include chemical and photo-sensing, computation, power generation, and active surface control.

Program Impact:

This is a highly collaborative program that is focused on a very complex task: the development and understanding of nanomachines tailored at the atomic level to control energy and information via mechanical processes. The primary motivation for this program is a desire to better understand the fundamental science that governs molecular scale machines, including energy transfer processes at the nanoscale, non-equilibrium dynamical properties, environmental and dissipative effects, and nanoscale manipulation of information. These activities directly address several DOE-BES grand challenges, including design of revolutionary new forms of matter with tailored properties, mastering of energy and information at the nanoscale, and characterization of matter away from equilibrium. This program has made significant impacts in areas such as electromagnetic molecular switching at surfaces, nanostructure conversion of heat to work, development of hybrid biosynthetic nanomachines, and nanostructure-based information management. These successes have been made possible through a highly collaborative effort coordinated through LBNL that involves six faculty scientists who together bring a combined set of skills that are collectively required by this program. These skills include organic and inorganic synthesis, single-molecule characterization of nanomachine elements at surfaces, characterization of single molecule biomachines, integration of molecular elements with patterned nanoelectronics, and theoretical modeling of molecular machine elements. The collaborative, multi-disciplinary research environment fostered by LBNL is critical to promoting the effective synergy that exists within this program.

FY 2009 Authorized Budget (New BA): $940k

Program Personnel Supported in FY2009:

Principal Investigators: M. Cohen 5%, J. Frechet 5%, S. Louie 5%
Postdoctorals: R. Maillard 80%, F. Giustino 5%, L. Berbil-Bautista 75%, V. Rodionov 40%, M. Loster 90%
Graduate Students: C. Hetherington 50%, V. Brar 30%, X. Zhang 30%, K. Ray 50%
Administrator: D. Tatum (55%)

Interactions:

Internal: National Center for Electron Microscopy, National Scientific Computing Center (NERSC), Advanced Light Source, Berkeley Microfabrication Laboratory
External: IBM Almaden, Yale, University of Vienna, Max Planck Institute Stuttgart, University of Pennsylvania, Pennsylvania State University, UCLA, SUNY Stony Brook, Seoul National University, Korea, Hong Kong University of Science & Technology, and Universidad del Pais Vasco, Spain.

Related Project URL: http://physics.berkeley.edu/research/crommie/

FWP Title: Nanowire-based Functional Devices and Assemblies **Name of the Laboratory: LBNL**
FWP Number: KC1204 **B&R Code: KC020103**

Program Abstract:

The goal of this research is to develop the science and technology of a broad spectrum of 1-dimensioanl inorganic semiconducting nanostructures or nanowires. *The main focus of the program is on the synthesis, assembly/integration of inorganic nanowires and the investigation of fundamental optical properties of these nanostructures.* Our synthetic approach relies on a powerful chemical synthesis technique, vapor-liquid-solid (VLS) process that can be used to grow monocrystalline semiconductor nanowires and their alloys. We have gained excellent control over nanowire size and aspect ratio; growth orientation, position and density. Methods for making complex heterojunctions and alloy semiconductor nanowires or nanotubes are also being developed. In addition, solution methods are also being investigated in order to synthesize nanowires with sub-2 nm diameter. Both parallel process (Langmuir-Blodgett and dip-coating technique) and serial process (nanomanipulation, optical trapping) are being explored for the hierarchical assembly of these nanowire building blocks for their potential nanophotonic and other applications. Finally we are actively investigating the fundamental optical properties of these semiconductor nanostructures including for example non-linear optical mixing, lasing and waveguiding, bandgap and bandedge of the newly-developed InGaN semiconductor nanowires.

Program Impact:

Semiconductor nanowires have witnessed an explosion of interest in the last several years due to advances in synthesis and the unique thermal, optoelectronic, chemical, and mechanical properties of these materials. The potential applications of single-crystalline nanowires are truly impressive, including computational technology, communications, spectroscopic sensing, alternative energy, and the biological sciences. In the context of global energy needs, low-cost solution-phase nanowire synthesis has also sparked interest in novel solar cell architectures which may play a significant role in the renewable energy sector. Additionally, the use of compact, integrated optical sensors can be envisioned for the detection of pathogenic molecules in the arena of national security or for the diagnosis and study of human disease. This breadth of application naturally requires a multidisciplinary community, including but not limited to materials scientists, chemists, engineers, physicists, and microbiologists, all converging to solve challenging optical problems at nanometer length scales. However, the materials must be synthesized and characterized before the exploration of their properties and applications can take place.

The goal of this multidisciplinary research is to systematically develop the science and technology of a broad spectrum of such 1-dimensional inorganic semiconducting nanostructures. For any of the potential nanowire applications such as photonics and energy conversion, it is important to gain fundamental understanding of their optical properties. Hence, another important aspect of the current efforts is to explore the fundamental optical properties of these semiconductor nanostructures including for example non-linear optical mixing, lasing and waveguiding, bandgap and band-edge of the newly-developed InGaN semiconductor nanowires as well as the oxide superlattice nanowires.

FY 2009 Authorized Budget (New BA): $411k

Program Personnel Supported in FY2009:

Principal Investigator: P. Yang 10%
Postdoctoral Fellows: J. Beeman 5%, J. Cao 20%
Graduate Students: M. Moore 40%, C. Liu 5%, C. Hahn 20%
Administrator: L. Garcia 50%

Interactions:
Impacting collaborations:
BES program Organic-Inorganic Nanocomposites (KC3104): Nanowires of suitable compositions could be used in this program.
BES program Nanostructured Thermoelectrical Materials (KC 1205): Leveraging thermoelectrical characterization within the program.

FWP Title: Nanostructured Materials for Thermoelectric Energy Conv. Name of the Laboratory: LBNL
FWP Number: KC1205 B&R Code: KC020103

Program Abstract:
Direct thermal to electrical energy conversion using solid-state thermoelectric devices is attractive because such devices contain no moving parts and are environmentally benign. Such devices, however, are not widely used because their performance is below 10 percent of the Carnot limit due to lack of adequate materials. While five decades of research has led to understanding of the basic attributes of a bulk thermoelectric material, there is no clear roadmap of increasing from 1 to 3. The challenge lies in the fact that the thermopower, *S*, electrical conductivity, *s*, and thermal conductivity, *k,* are interdependent making optimization extremely difficult. Recent research on nanostructured materials has led to sharp increases in *ZT*. As part of this project, we have begun uncovering some of the underlying reasons, based on which we have created a set of criteria for designing nanostructured thermoelectric materials. Based on these criteria, we are exploring three new classes of nanostructured materials: (i) molecular heterostructures; (ii) complex oxides; (iii) bulk nanostructured semiconductors. We lay out the reasons of why these materials have promise for increasing *ZT* and outline a comprehensive approach for materials synthesis, various forms of characterization, as well as theory and modeling.

Program Impact:
Peidong Yang's expertise on inorganic nanomaterials synthesis is critical to this program. He will focus on inorganic synthesis of Group IV nanomaterials. Ramesh Ramamoorthy will bring his experience and knowledge on complex oxides and will focus on creating nanostructured complex oxides for thermoelectric applications. Joel Moore will carry out theoretical modeling of electron and phonon transport that is critical to the success of the program. Rachel Segalman will bring her experience in organic synthesis and transport measurement to study organic-inorganic heterostructures. Jeff Urban's, a new co-PI in this program, expertise in solution processing will be leveraged for spin-coated thermoelectrics as well as organic-inorganic nanostructures. The graduate students and post-docs will essentially be "glue" personnel and will be jointly supervised by all of us, but with each student or postdoc having emphasis on one area. In the short period of 3 years since its inception, this program has already had significant impact at multiple levels. We have formed a highly interactive team of scientists focused on advanced materials synthesis, thermal and electrical transport studies and theoretical methods to probe the phenomena. Several key papers in the highest impact journals have resulted from this research. This is also a well-balanced program that is rooted in the basic thermal transport physics of artificially engineered nanostructures, but with a keen eye on the potential to transform the thermal-to-electrical energy conversion landscape. In this regard, the work in this program has led to the formation of a start-up company, Alphabet Energy, that is focused on commercializing the successful demonstration of large ZT in Si nanowires.

FY 2009 Authorized Budget (New BA): $740k

Program Personnel Supported in FY2009
Principal Investigators: R. Ramesh 10%, J. Moore 10%
Postdoctorals: R. Chen 60%, S. Mukerjee 40%, K. See 100%
Graduate Students: S. Andrews 20%, J. Lim 10%, X. Gu 20%, M. Scullin 30%, J. Kardel 10%, A. Chari 5%, J. Malen 40%
Technical Staff: J. Tang 20%, P. Murphy 20%

Interactions:
This is a joint project between Ramamoorthy Ramesh (PI), Joel Moore, Peidong Yang, Rachel Segalman and Jeff Urban. There are also collaborations with NCEM, Molecular Foundry, ALS. We also collaborate extensively with scientists at other NL's and academic institutions.

FWP Title: Spin Functionality through Complex Oxide Heteroepitaxy **Name of the Laboratory: LBNL**
FWP Number: KC1206 **B&R Code: KC020103**

Program Abstract:

This program is focused on a *strategic materials issue* associated with the increasing demand for new electronics from energy, information and national security technologies: the development of oxide thin films and heterostructures with spintronic functionality. Atomically precise complex oxide thin films and heterostructures with magnetic functionality comprise a new class of oxide materials that may form the basis for the development of a more energy efficient spin-based electronics. Therefore from a fundamental materials perspective as well as a technological perspective, this research is relevant to the DOE BES mission. Complex oxides exhibit a wide range of magnetic, electronic and optical properties that can be tuned by parameters such as lattice strain and chemical substitution. The tunability of their structure and properties, make them ideally suited for the development of novel thin films and heterostructures with magnetic or spin polarized functionality. More specifically we (i) design and synthesize complex oxide materials with new magnetic functionality (ii) obtain a fundamental understanding of the nature of magnetism by developing and characterizing novel magnetic ground states in oxide thin films and heterostructures and (iii) develop close collaborations with colleagues at LBNL and other DOE labs; (iv) act as a resource for thin film materials development and (v) train the next generation of scientists in thin film materials synthesis.

Program Impact:

The development of new complex oxide thin films and hetereostructures with magnetic functionality has both impact on our fundamental understanding of magnetism as well as the technological viability of this class of materials in more energy efficient electronics applications. These materials provide model systems that shed light on the nature of magnetism at boundaries of magnetic materials. Understanding magnetism at these surfaces and interfaces is a key element in the development of a more energy efficient spin-based electronics. This program has extensive collaborations, as listed below, with colleagues at LBNL and other institutions and enables other DOE research programs by providing novel materials.

FY 2009 Authorized Budget (New BA): $250k

Program Personnel Supported in FY2009:

Principal Investigator: Y. Suzuki 10%
Graduate Students: A. Grutter 50%, V. Mehta 40%

Interactions:

Elke Arenholz, Andreas Scholl (Advanced Light Source, Lawrence Berkeley National Laboratory)
Bruce Harteneck (Molecular Foundry/ Lawrence Berkeley National Laboratory)
Peter Fischer, Jeff Kortright, Andreas Schmidt, Kin Man Yu (Materials Science Division/ Lawrence Berkeley National Laboratory),
Michael Toney (SLAC Nationall Accelerator Laboratory)
Miaofang Chi, Nigel Browning (UC-Davis)
Chang Beom Eom (University of Wisconsin at Madison)
Arturas Vailionis (Stanford), Bud Bridges (UC Santa Cruz)
Nicola Spaldin (UCSB)

FWP Title: Sub-wavelength Metamaterial Design, Physics & Application **Name of the Laboratory: LBNL**
FWP Number: KC12XZ **B&R Code: KC020103**

Program Abstract:
Metamaterials enable the realization of novel physical properties that are unattainable from natural materials. Theoretical and preliminary experimental studies have shown that it is possible to make electromagnetic metamaterials with unprecedented characteristics such as left-handedness with simultaneous negative permittivity and permeability, perfect lens that focus electromagnetic waves far below the diffraction limit, and artificial magnetism from nonmagnetic materials. However, the research in optical metamaterials is rather limited due to the fundamental challenges in physical science, materials physics and characterizations. To address these critical challenges, this project sets to explore novel optical metamaterial physics. In particular, is it fundamentally possible to have a 3D far-field optical lens with diffractionless imaging resolution by recovering evanescent waves through a negative index medium? We believe that the fundamental discoveries from this project will have profound impacts on a wide range of applications such as nanolithography, sub-diffraction limited optical microscopy, high speed optical communications and nanophotonics for energy conversion with high efficiency.

Program Impact:
The accomplishment of this project will enable a new generation of optical materials with unprecedented properties and applications. It will have deep impact on the current optical technologies, such as optical imaging, nanophotonics, optical communications, and optical circuits. In addition, the novel nanofabrication and advanced characterization techniques involved in this program can be readily transferred to other DOE related programs.

The research draws cooperative efforts from multiple PIs and will be performed in three phases. In Phase I, Zhang (UCB and LBL) will devote time to the theory and modeling of 2D sub-diffraction hyperlens, such as to estimate the best polarization condition for the imaging. In Phase II, Zhang will be responsible for metamaterials sample fabrication at LBNL and UC Berkeley. Finally, in Phase III of the proposed work, various optical characterizations will be performed by Shen (UCB and LBL). Pendry (Imperial College) and Smith (Duke) plans to spend a month each year at LBNL to collaborate with the team.

FY 2009 Authorized Budget (New BA): $300k

Program Personnel Supported in FY2009:
Postdoctorals: H. Cang 40%, X. Yang 70%, X. Yin 100%

Interactions: We have strong interactions with various parties at LBL which are focusing on nano-optics, metamaterials and photonic crystals, including Stefano Cabrini (Molecular Foundry, LBL), Eli Yablonovitch (UCB and LBL) and Feng Wang (UCB and LBL), Mark Martin (ALS, LBL)

FWP Title: Nanocomposite Proton Conductors **Name of the Laboratory: LBNL**
FWP Number: KC13H **B&R Code: KC020103**

Program Abstract:

The program aims to design, synthesize and test rare earth phosphate materials for proton conducting applications in the temperature region of 300-450 degrees Celsius. The program relies on three major approaches: a theoretical understanding of proton conduction in rare earth phosphates employing quantum chemical computation and molecular simulation; the chemical design, synthesis, and proton conductivity measurement of nano-composite materials expected to exhibit facile proton conduction; and the structural and dynamical characterization of the nano-composite materials using a range of advanced characterization methods including nanoscale structural and chemical electron microscopy, vibrational and x-ray spectroscopy, and nuclear magnetic resonance (NMR). Aliovalently-substituted rare earth phosphates and rare earth phosphate glasses and glass/ceramics are being synthesized and tested for proton conduction. A comparison of theoretical predictions, observed conductivities, and spectroscopic analyses provides an insight into nature of conduction at the atomic level, and directs the synthesis of novel nano-composite rare earth phosphates.

Program Impact:

Achieving the program objectives requires the close collaboration of PI's with expertise in materials synthesis, structural, electrical, and electrochemical characterization, first principles calculations, nuclear magnetic resonance, electrochemical interface processes, and photoelectron spectroscopy.
When successful, this research will form the basis for a new class of materials for of hydrogen fuel cells that relieve some of the drawbacks of other fuel cell systems.

FY 2009 Authorized Budget (New BA): $850k

Program Personnel Supported in FY2009:

Principal Investigators: L. DeJonghe 20%, J. Reimer 10%, P. Ross 10%
Postdoctorals: R. Wang 100%, G. Zhang 100%, J. Feng 20%
Graduate Students: N. Adelstein 30%, J. Stettler 30%
Undergraduate Students: H. Ray 5%, G. Ye 10%
Technical Staff: M. Tucker 30%

Interactions:

J. Neaton LBNL-Molecular Foundry
V. Radmilovic LBNL- NCEM

FWP Title: Studies of Hybrid Biomolecular Materials with Scattering… **Name of the Laboratory: LBNL**
FWP Number: MS801 **B&R Code: KC020201**

Program Abstract:

Synthetically modified biomolecules provide a powerful set of building blocks for the construction of complex nanoscale materials. The key advantage of this approach lies in the ability of the rigidly-defined structures to order multiple functional components through efficient self-assembly processes. Structural characterization of the resulting materials is essential to both improve our fundamental understanding on this new family of building blocks and to assemble them into functional biomolecular materials. This program will carry out structural analysis of biomolecular assemblies on multiple length scales. Two families of bio-inspired building blocks, *de novo* designed helix bundle peptide-polymer conjugates and chemically modified viral capsids, will be accessed using site-specific protein modification reactions. Through the use of scattering "tags", two new viral capsid assembly strategies will also be developed. After the attachment of polymers and metal complexes, the hybrid structures will be assembled to yield materials in solution or as thin films. X-ray (soft and hard) and neutron scattering techniques will then be used for the systematic characterization of the structure and phase behavior of these materials. Scattering techniques using soft X-rays will be developed in this program to investigate the assembly of peptide/protein containing materials. Specifically, the nanoscale organization of peptide-containing biomolecular materials in solution, in thin films and at interfaces will be investigated. The outcome of these studies will be a powerful new suite of characterization tools, along with critically important insights for the design of future materials through biomolecular self-assembly.

Program Impact:

This program carries out structural studies on the hierarchical assemblies of two families of biomolecular building blocks, *de novo* designed helix bundle peptide-polymer conjugates and chemically engineered viruses. Synthetic routes will be developed to synthesize peptide-polymer conjugates with well-defined architectures and viruses with site-specific protein modification. Various scattering techniques using synchrotron and neutron sources will be used to elucidate the assemblies at multiple length scales with a focus to obtain fundamental understanding on the phase behavior of peptide/protein and polymers and the parameters dictating the assembly process. Soft X-ray scattering techniques will be explored to study the nanostructures of peptide-containing biomolecular materials. Using *novo* designed photoactive peptide-polymer conjugate and chemically modified TMV as examples, the fundamental principles emerging from this program should be applicable to other building blocks and functionalities can be readily incorporated by varying building blocks. These research efforts will not only enrich our fundamental understanding in phase behavior of biomolecular building blocks, but also pave the path to generate functional materials with properties similar or superior to what seen in nature.

FY 2009 Authorized Budget (New BA): $500K

Program Personnel Supported in FY2009:

Principal Investigators: T. Xu 10%, B. Jerome 30%, J. Kortright 5%
Postdoctorals: A. Presley 100%, M. Valvidares 70%
Graduate Students: M Dedeo 30%, N. Dube 5%, S. Liu 10%, J. Shu 5%

Interactions:

- Xu/Frances: develop synthetic routes to prepare peptide-polymer conjugates with well defined architecture
- Xu/Kortright: use resonant soft X-ray scattering techniques to study peptide-polymer conjugates in thin films
- Kortright/Frances: develop soft X-ray scattering techniques using metal-tagged virus particles
- Frances/Xu: structural characterization of virus nanoparticles using hard X-ray and neotron scattering
- Kortright/Xu: initial exploration on using polarized soft X-rays to characterize peptide secondary structure
- Jérome/Kortright: develop reflectivity techniques to characterize polymer chain orientation in thin films using polarized soft X-ray

FWP Title: Ultrafast Materials Science **Name of the Laboratory: LBNL**
FWP Number: KC2203 **B&R Code: KC020201**

Program Abstract:

This research program applies advanced ultrafast techniques to fundamental problems in condensed matter physics. Present focus is on (i) complex materials where correlation among charges and between charge, spin, and phonons lead to new properties, quasiparticles, and exotic phases; and (ii) novel physics at surfaces, interfaces, and in nanostructured materials. Ultrafast spectroscopy provides new insight by separating correlated phenomena in the time domain with resolution shorter than the underlying coupling processes. Ultrafast technology also provides the foundation for surface and interface specific nonlinear spectroscopies for probing complex materials. The program consists of four coupled and complementary research areas: (1) understanding charge, spin and quasiparticle dynamics in highly correlated systems using THz spectroscopy and time-resolved four-wave mixing, (2) understanding magnetization dynamics in correlated materials using transient spin grating and time-resolved magneto-optic Kerr spectroscopy, and (3) understanding photo-induced cooperative phase transitions, critical phenomena, and electron phonon coupling in novel materials and molecular crystals using ultrafast visible and mid-IR spectroscopy. The new (fourth) component of this research program will apply ultrafast X ray spectroscopy and VUV/EUV angle-resolved photoemission spectroscopy to understand the dynamics of atomic structure and valence electronic structure in complex materials. Measurements of correlated phenomena on fundamental time scales, at atomic spatial scales, with momentum resolution and element specificity are indispensable for achieving new insight onto the emergent physics of complex materials, nanostructures, and novel states of matter.

Program Impact:

This program has generated new fundamental knowledge of electronic and atomic dynamics in condensed matter. Results from semiconductors, correlated electron systems, nanostructures, surfaces, and molecular complexes have challenged previously held assumptions and advanced new paradigms to describe the dynamic behavior that underpins novel material properties and functionality. The technical and scientific complexity of the challenges addressed in this program requires a multi-investigator effort. The combination of state-of-the-art ultrafast laser facilities, femtosecond x-ray beamlines, photoelectron spectroscopies, and precision ultrafast measurement techniques covering a very broad range of the electromagnetic spectrum, from THz to X-rays, are beyond what could be achieved in a single-investigator effort. They substantially leverage the personnel, synergistic expertise, and resources of a national laboratory and the ALS as a national user facility.

FY 2009 Authorized Budget (New BA): $1019k

Program Personnel Supported in FY2009:

Principal Investigators: R. Schoenlein 10%, R. Kaindl 90%,
Postdoctorals: S. Zhao 10%, M. Langner 20%, H. Choi 100%, J. Robinson 25%, J. Koralek 30%, J. Seidel 20%, M. Rini 40%
Graduate Students: Y. Zhu 30%, I. Cotoros 10%, M. Langner 20%, L. Yang 20%,
Undergraduate students: B. Jaeck (DAAD/IGERT), M. Tanksalvala (SULI).

Interactions:

Internal: LBNL Materials Science Div. incl. Molecular Foundry, Chemical Sciences Div., Advanced Light Source.
External: U.C. Berkeley Physics Dept., U.C. Berkeley Chemistry Dept., U.C. Berkeley EECS Dept., Stanford Univ., U.C. Santa Barbara, U.C. San Diego, Washington State U., Oxford U., CFEL DESY Hamburg, Univ. Illinois Urbana-Champaign, Notre Dame Univ., Naval Res. Lab., U. British Columbia, U. Tokyo, Tokyo Inst. Tech., CRIEPI Japan, Ecole Normale Superieure de Paris, Weizmann Inst.

Related Project URL: http://www.lbl.gov/msd/programs/3si/1.1uf.html

FWP Title: Superconductivity **Name of the Laboratory: LBNL**
FWP Number: KC2201 **B&R Code: KC020202**

Program Abstract:

The program combines two projects concerned with superconductivity: (1) the fundamental science and development of Superconducting QUantum Interference Devices (SQUIDs) and their application to ultrasensitive measurements; and (2) research on phase coherence in superconductors and the superconductor-insulator phase transition in two dimensions. Much of the research on SQUIDs is focused on achieving the quantum limit of detection for applications ranging from a search for the axion to the readout of superconducting quantum bits. SQUIDs with submicrometer dimensions—so called NanoSQUIDs—are being developed to study single molecule magnets (SMMs), which have magnetic moments of a few Bohr magnetons. Measurements of the dynamics of these molecules, for example the longitudinal and transverse relaxation times T_1 and T_2, require a time resolution of 100 ns or less, which is accomplished with a nondissipative, dispersive readout scheme. The origin of l/f flux noise in SQUIDs at low temperatures is investigated theoretically and experimentally. Recent theoretical work in collaboration with Louie and Lee suggests that the noise originates in the metal-induced gap states that give rise to localized states at the disordered interface between the superconductor and the substrate. These localized states also produce paramagnetism. A low-temperature superconducting scanning tunneling microscope (S-STM) with a superconducting tip is used to probe the superconducting order parameter in unconventional superconductors on the scale of the coherence length. The S-STM is also used to study spatial variations of the Cooper pair density in the fluctuating regime of the superconductor-insulator phase transition in quench-condensed two-dimensional films.

Program Impact:

The SQUID amplifier developed under this program is installed on the axion detector at LLNL, and will ultimately improve its scan rate by 2 – 3 orders of magnitude. The SQUID multiplexer originally developed under this program was engineered by other groups at LBNL and UCB, and is now in operation on telescopes at Atacama, Chile and on Antarctica in searches for galaxy clusters. Joint projects within this program include the installation of a SQUID to increase the sensitivity of a scanning tunneling microscope used to study phase coherence in high-transition temperature superconductors, and the study of large arrays of Josephson junctions patterned in the Molecular Foundry. The theory of localized electron states at disordered superconductor-insulator interfaces, in collaboration with S.G. Louie and D-H. Lee, explains the quarter-century old problem of low frequency noise in SQUIDs, and suggests that highly ordered interfaces should be free of such noise. Ultimately, elimination of this noise may lead to longer decoherence times in superconducting qubits. A new direction, in collaboration with I. Siddiqi, is the development of ultrasensitive "nanoSQUIDs" to study single-molecule magnets supplied by J.R. Long at MSD. This study will address some of the Grand Science Challenges posed by Basic Energy Sciences, specifically "How do remarkable properties of matter emerge from the complex correlations of atomic or electronic constituents and how can we control these properties?" and "How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?"

FY 2009 Authorized Budget (New BA): $560,000

Program Personnel Supported in FY2009

Principal Investigator: J. Clarke 10%
Technical Staff: Shane Cybart 50%
Graduate Students: S. Anton 5%, Michael Hatridge 20%, Nathan Kelso 50%, I. Lee 20%, S. O'Kelley 10%
Administrator: B. Salisbury 80%

Interactions:

D. Kinion, A. Lanzara, D-H. Lee, S.G. Louie, S. Ono, J. Orenstein, A. Pines, R. Ramesh, I. Siddiqi

FWP Title: Quantum Materials **Name of the Laboratory: LBNL**
FWP Number: KC2202 **B&R Code: KC020202**

Program Abstract:
Quantum physics provides the theoretical basis for our understanding of the electronic properties of *all* materials. However, there exists a fascinating sub-class of condensed matter systems, now widely known as "*quantum materials*," in which quantum mechanics plays an especially profound role in determining the nature of macroscopic order parameters and the phase-transitions between them. In some cases, such as supeconductors, this occurs because the order parameter is explicitly a quantum mechanical object. In many other such systems, quantum effects dominate the physics because of the interplay between competing order, frustration, strong interactions, and low-dimensionality. These systems display a marvelously rich and diverse range of physical phenomena. Transition metal oxides, *e.g.,* manganites, cuprates, ruthenates and cobaltates, are systems whose interacting charge, spin, orbital, and lattice degrees of freedom exemplify the diversity of quantum materials.

Program Impact:
It is universally recognized that the scale of the quantum materials problem requires a team-oriented, rather than individual PI, approach. At LBNL we have brought together a team of researchers with strongly overlapping interests in transition metal oxides (and related systems) and synergistic capabilities. Our Quantum Materials Group was first organized in Fall 2006 as a unified FWP. The team members and their research specialties are illustrated in the figure to the left. Our group includes experts in the theory of strongly correlated systems (Lee, Vishwanath), bulk crystal synthesis (Birgeneau, Bourret), thin-film synthesis (Ramesh), and characterization (Birgeneau, Dynes, Lanzara, and Orenstein). We bring to bear powerful experimental tools (transport, photoemission spectromicroscopy, optical spectroscopy, electron microscopy and spectroscopy, and neutron scattering) in conjunction with comprehensive theoretical approaches to understanding the complex phenomena that arise in quantum materials. With expertise in both single crystal and thin film growth, we are able to compare the properties of quantum phases in the bulk with those that occur in thin films and heterostructures. The work in this FWP is complemented by strategic collaborations with colleagues at other national labs, academic institutions as well as researchers around the world.

FY 2009 Authorized Budget (New BA): $1,368k

Program Personnel Supported in FY2009
Principal Investigators: Bourret-Courchesne 10%, D. Lee 10%, J. Orenstein 10%, R. Ramesh 10%, A. Vishwanath 20%
Postdoctorals: C. Rotundu 100%, S. Wilson 90%, Y. Ran 50%, Z. Yan 5%, C. Jozwiak 60%, J. Graf 80%, C. Hwang 100%, H. Yao 10%, J. Koralek 30%, M. Rossell Abrodos 50%, J. Seidel 80%, L. Martin 80%
Graduate Students: M. Holcomb 30%, L. Yang 5%, M. Langner 20%, M. Yong 50%, C. Smallwood 40%, D. Siegel 10%, D. Garcia 50%, G. Pinuellas 10%, A. Kim 40%
Technical Staff: C. Ramsey 10%, S. Hanrahan 5%

Interactions: The Quantum Materials program is highly leveraged in terms of interdisciplinary collaborations within LBNL as well as outside (i.e., other national labs and academic institutions). A significant component of our research will be carried out in collaborations with scientists at the ALS (for example Lanzara and Ramesh will work with Rotenberg to carry out insitu studies of surface and interface electronic structure in complex oxide heterostructures); Lanzara is a key member of the ALS user community as well as formulating the future directions of this facility (for example, Lanzara is currently collaborating with Dr. Hussain (ALS), Dr. Lebedev (ALS) and Dr. Schmid (NCEM) for the development of a novel analyzer for spin ARPES). Lanzara and Ramesh are key users of various beamlines at the ALS for magnetic studies of complex oxide heterostructures and nanostructures as well as spectroscopy and collaborate extensively with Scholl, Arenholz, Rotenberg, Kortright and Fischer. We also have strong collaborations with scientists at the NCEM (Dahmen, Browning, Kieselowski, Schmid), in the area of energy loss spectroscopy and high resolution imaging of interfaces.

FWP Title: Magnetic Materials **Name of the Laboratory: LBNL**
FWP Number: KC2204 **B&R Code: KC020202**

Program Abstract:

Part (B) of the Nanoscale Magnetic Materials program at LBL supports part (A) by providing soft x-ray nanoscale imaging of magnetic materials at the XM-1 full field microscope, ALS beamline 6.1.2. The goal is to support day-to-day magnetic imaging at a spatial resolution of 20 nm while pursuing improved resolution approaching 10 nm and beyond. Currently the microscope has achieved 12 nm, a recently published world record. Achievement of 10 nm spatial resolution is tantalizingly close and hopefully will be achieved as microscope upgrades are completed in mid – FY10.

Program Impact:

This program is significantly impacting state-of-the-art knowledge of the properties of nanoscale magnetic materials, as evidenced by several publications in high profile journals and the large number of invited conference presentations by Peter Fischer (14). The program also has significant impact on worldwide goals and understanding of the challenges associated with achieving sub-10 nm spatial resolution for magnetic materials, as well as the broader range of scientific opportunities at this spatial scale. This work consistently provides the gold standard in nanoscale imaging. Extension of the picosecond studies to femtosecond temporal resolution is highly desirable, but is beyond the present level of support.

FY 2009 Authorized Budget (New BA): $2,405k

Program Personnel Supported in FY2009: (%FTE)
Principal Investigators: C. Fadley 50%, D. Attwood 15%, J. Kortright 80%
Scientific Staff: P. Fischer 40%, M. Im 40%, E. Anderson 30%, W. Chao 40%, J. Gamsby 15%, E. Gullikson 20%, R. Tackaberry 15%, H. Lee 50%, D. Hilken 40%, R. Gunion 30%
Administrators: J. Jones, S. Lai total 55%
Students: total 180%

Interactions:

The development of soft x-ray optics and a well engineered microscope are closely coupled to the study of magnetic materials properties as described in part A of this proposal. Support for general users of the microscope at the ALS is supported by BES/Scientific User Facilities through a separate account with the ALS. Zone plate structures for other BES supported microscopes at the ALS (three scanning transmission soft x-ray microscopes) are also funded by BES/Scientific User Facilities through a second account at the ALS. Zone plates for biomicroscopy at the NIH/DOE full-field microscope (XM-2) are funded separately by the NIH and DOE/OBER. Zone plates for other facilities, such as the Swiss Light Source, Canadian Light Source, Pohang Light Source, and any others outside Berkeley, are contracted on a full cost recovery basis. Support for zone plates and other nanostructures used in the development of applications with compact soft x-ray sources, such as laser high harmonic generation (HHG) and EUV/Soft x-ray lasers, is funded through a grant with the National Science Foundation (NSF). The NSF also supports graduate students who frequently contribute to the work in both sections A and B of this proposal. This includes the study of vortex motion in nanomagnetic structures, and the development of new phase contrast imaging and depth of field extension techniques, both recently demonstrated with the XM-1 microscope. In addition, efforts to enlarge the capability for the study of classes of epitaxially grown magnetic materials, such as complex oxides, using transmission soft x-ray microscopy have been pursued through the development of back-etching techniques for a variety of materials, including LSMO/STO and MgO. At some point it would be desirable that these efforts evolve from NSF student/postdoc support to DOE/BES support. Efforts to extend temporal studies of nanomagnetic structures from the present 70 psec to future fsec time resolution are presently unfunded, however preliminary work on concepts and requisite optical components (zone plate lenses and other soft x-ray diffractive structures, broadband and chirped multilayer mirrors, etc.) have begun as student projects.

FWP Title: Development of New Classes of Hydrogen Storage Materials **Name of the Laboratory: LBNL**
FWP Number: KC2205 **B&R Code: KC020202**

Program Abstract:
The Berkeley Hydrogen Storage Program consists of a broad-based, multi-investigator effort for developing fundamentally new types of hydrogen storage materials. Our approach is to explore numerous possibilities for new materials, and narrow our focus as the research progresses. Our effort focuses on the development of new nanostructured materials of potential utility in hydrogen storage applications. Specific areas of investigation include: the synthesis of new nanostructured boron nitride materials for comparison with carbon-based analogues, computational work leading to the prediction of structures with a high affinity for H_2, synthesis and evaluation of hydrogen uptake in magnesium-based nanocrystals, and the development and characterization of nanocrystal/metal-organic framework hybrid materials exhibiting room-temperature hydrogen uptake via a spillover mechanism. A hydrogen storage characterization facility containing one gravimetric and two volumetric high-pressure adsorption analyzers is maintained in order to provide accurate and immediate feedback on the properties of the many new materials generated. Ultimately, this research is expected to yield materials and science of potential value for enhancing the range of hydrogen fuel cell-powered vehicles.

Program Impact:

This research is intended to generate fundamentally new types of hydrogen storage materials with the potential for meeting the criteria required for making hydrogen fuel cell-powered vehicles feasible. In particular, materials with the potential for attaining a reversible uptake of 6 wt % H_2 while operating at moderate temperatures and pressures are sought. The synergy of many scientists in one location working toward a common goal is expected to accelerate our progress and lead to new ideas via cross-fertilization.

FY 2009 Authorized Budget (New BA): $550k

Program Personnel Supported in FY2009:
Principal Investigators: J. Urban 5%, J. Long 10%
Postdoctorals: H. Choi 30%, H. Lee 50%, H. Moon 90%, M. Tang 70%, T. Gupta 20%
Graduate Students: Z. Herm 20%, T. McDonald 5%, J. Rinehart 5%, K. Sumida 10%, B. Wiers 10%, J. Zadrozny 10%, K. Erickson 30%

Interactions:

Collaborative efforts with Dr. Craig Brown of NIST have been undertaken to probe hydrogen adsorption within metal-organic frameworks via neutron powder diffraction.

FWP Title: Novel sp2-Bonded Materials and Related Nanostructures **Name of the Laboratory: LBNL**
FWP Number: KC2207 **B&R Code: KC020202**

Program Abstract:

Ab-initio quantum mechanical calculations to predict new materials structures and relate them to electronic structure and mechanical and thermal properties. Experimental synthesis of novel sp2-bonded materials including functionalized nanostructures, and characterization using SEM, TEM, STM, AFM, XRD, photoemission, mechanical properties, and transport properties. Nanoscale device fabrication and testing. Strong connection between theory and experiment.

Program Impact:

This interdisciplinary program combines expertise in chemistry, biology, experimental condensed matter physics, and theoretical materials physics. The program has made significant impact in the fields of atomic scale characterization of materials, including TEM imaging static and dynamic configurations of light atoms and molecules and STM determination of local electronic structure of graphene. These experimental studies relied on coordinated and fully integrated theoretical investigations. BN nanotubes produced by the materials synthesis effort of this program were subsequently functionalized for specific biological activity using state-of-the-art chemical biology methods. This collaboration again yielded spectacular results which could not have been achieved through uncoordinated single-investigator studies. Solar cells were fabricated and characterized via collaborations between polymer chemists and solid state physicists; these cells have shown promising voltage characteristics. All of the above successes have direct relevance to the DOE mission.

FY 2009 Authorized Budget (New BA): $1,000k

Program Personnel Supported in FY2009:

Principal Investigators: A. Zettl 20%, Cohen 5%, Louie 5%
Postdoctorals: H. Lee 30%
Graduate Students: B. Belardi 30%, X. Zhang 20%, C. Park 30%, D. Okawa 30%, K. Erickson 5%, C. Girit 50%, B. Kessler 50%, M. Rousseas 40%
Administrators: G. Lang 75%, K. Carkhuff 10%

Interactions: (limit to current interactions and collaborations)
Internal: Molecular Foundry, National Center for Electron Microscopy, National Scientific Computing Center (NERSC), Advanced Light Source, Berkeley Microfabrication Laboratory
External: CNRS France, University of Vienna, Max Planck Institute Stuttgart, University of Pennsylvania, Pennsylvania State University, UCLA, SUNY Stony Brook, Seoul National University, Korea, Hong Kong University of Science & Technology, and Universidad del Pais Vasco, Spain

FWP Title: Condensed Matter Theory **Name of the Laboratory: LBNL**
FWP Number: KC2301 **B&R Code: KC0202030**

Program Abstract:

This program aims to understand and compute material properties and behaviors. Novel materials and new concepts are explored. A variety of theoretical techniques are employed, ranging from first-principles electronic structure calculations to new conceptual and computational frameworks suitable for complex materials/nanostructures and strongly interacting electron systems. One emphasis is to investigate realistic systems employing microscopic first-principles approaches. Model systems are also examined. Studies include bulk materials, nanostructures, superconductors, surfaces and interfaces, and reduced-dimensional systems. Close collaboration with experimentalists is maintained. Another emphasis is to push the frontier of theory beyond the Landau paradigm toward a framework capable of describing and predicting the behavior of strongly correlated systems. Through interaction with experiment, new phases, new phase transitions, and new organization principles may be discovered. Equally important is the development of computational methods suitable for increasingly complex materials and strongly correlated materials.

Program Impact:

This is a broad-based program involving 3 principal investigators of different expertise and covering two complementary efforts: 1) quantum theory of materials, and 2) strongly correlated electron systems. The program has very strong ties with other programs within the Lawrence Berkeley National Laboratory (LBNL), in particular with the diverse experimental efforts, allowing timely and synergetic interactions. The resources at LBNL also make possible the long-term development of large-scale computer codes for simulation of complex phenomena and systems. The research strives to have impact on several of the grand challenge areas of DOE-BES, including designing new form of matter with tailored properties, mastering energy and information at the nanoscale, controlling material processes at the level of electrons, and understanding emergent properties from complex correlations of the atomic or electronic constituents. Studies have led to discoveries of new materials, nanostructures, and properties; explanation of experiments; and development of new theoretical and computational methods.

FY 2009 Authorized Budget (New BA): $334K

Program Personnel Supported in FY2009:
Principal Investigators: M. Cohen 5%, D. Lee 5%, S. Louie 5%
Postdoctorals: H. Lee 30%, H. Zhai 70%
Grad students: J. Noffsinger 10%, B. Malone 10%;
Administrator: K. de Raadt 80%

Interactions:
There are strong interactions among the condensed matter theorists in the Materials Sciences Division, which include Cohen, Louie, Lee, Vishwanath, Moore, L.-W. Wang and Souza. Collaborations with theorists in the Molecular Foundry include J. Neaton and D. Prendergast. Current collaborations with experimentalists include the groups of A. Zettl, M. Crommie, F. Wang, J. Frechet, J. Clarke, A. Lanzara, E. Rotenberg, J. Tilley, D. Stamper-Kurn, and I. Siddiqi. Interactions with external institutions include Georgia Tech, U of Texas at Austin, Tokyo Inst.of Techn. (Japan), Seoul National U. (South Korea), Korea Institute of Advanced Study (South Korea), Yonsei U. (South Korea), IU. Pais Vasco (UPV/EHU, Spain), National Taiwan U (Taiwan), KITP (Beijing, China), Fudan U. (China); Center for Advanced Study (Tsinghua U., China).

FWP Title: Charge Patching Method for Electronic Structures & Charge… Name of the Laboratory: LBNL
FWP Number: KC2303 B&R Code: KC0202030

Program Abstract:
The goal of this project is to develop new methods to calculate the electronic structures, optical properties and charge transports of large organic, inorganic and organic/inorganic mixture systems. This will extend our capability of calculating such systems in ab initio accuracy from a few hundred atoms to hundreds of thousands of atoms. This project continues to develop the charge patching methods (CPM) for organic and inorganic systems. It also develops other linear scaling methods, especially the linear scaling three dimensional fragment (LS3DF) method. It studies the structure-to-property relationship for organic systems, ligand passivation of inorganic nanocrystals, organic/inorganic interface, large inorganic systems like nanocrystals and alloys. For organic systems, it studies polymers and organic small molecules. It studies the carrier transports in organic systems. In the long term, it also plans to test the CPM for evaluating the non-bond interactions in force field models.

Program Impact:
Organic polymers and organic/inorganic mixed systems often contain tens of thousands of atoms. For a long time, there had no ab initio accuracy method capable of calculating their electronic structures and carrier transport properties. As these systems are used more and more for electronic devices, solar cells, and batteries, it is imperative to calculate their electronic structures, and understand the structure-to-property relationships. This is especially true for modeling the realistic complex systems used in experiments, instead of a single ideal polymer chain as often done in many theoretical investigations. The current project combines a general charge patching approach developed in this group with large scale computations provided by the national lab facilities. The combined approach allows the simulation of large organic, and organic/inorganic systems directly relevant to experiments. It also changes the field from an empirical and phenomenological model based paradigm to an ab initio calculation based paradigm. Setting in the national Lab environment, it allows the PIs to collaborate closely with other experimental projects, and with computer scientist and mathematicians to develop large scale computational codes (e.g., the LS3DF code).

FY 2009 Authorized Budget (New BA): $275k

Program Personnel Supported in FY2009:

Principal Investigator: LW Wang 10%
Postdoctorals: S. Dag 90%, N. Vukmirovic 90%

Interactions:
Miquel Salmeron, Material Science Division, Lawrence Berkeley National Laboratory, for surface molecular attachment; Wanli Yang, Advanced Light Source, Lawrence Berkeley National Laboratory, for electronic structure of polymer electrode for battery; Andrew Canning, Computational Research Division, Lawrence Berkeley National Laboratory, for large scale LS3DF code development;Jose Manuel Roldan, Univ. Jaen, Spain, for electronic structure calculations of their special polymer systems; Yong Zhang, Univ. North Carolina, Charlotte, for apply charge patching model for alloy electronic structure calculations.

FWP Title: Chemical and Mechanical Properties of Surfaces, Interfaces… Name of the Laboratory: LBNL
FWP Number: KC3101 B&R Code: KC020301

Program Abstract:
The purpose of this program is to carry out atomic level studies of surfaces and nanomaterials, focusing on chemical, mechanical and physical properties: structure, diffusion, reactions, catalysis, friction and wear. The molecular level knowledge generated by the proposed studies will help the development of novel catalysts with higher activity and selectivity and the discovery of novel materials of nanometer dimensions with unique mechanical, chemical and optical properties, and of materials with improved mechanical properties of adhesion, friction, and wear. The results from this project benefits many energy based industries, including chemical, petroleum, mechanical, electronics, solar energy, etc. To accomplish these goals we utilize materials in the form of single crystals, biointerfaces and nanoparticles. We develop methods for making nanocrystals with narrow particle size distribution and well-defined shape. We develop new instrumentation for the characterization of our materials under the widest possible range of operating conditions: under vacuum, at ambient pressure and at the solid-liquid interface. These include sum frequency generation (SFG) surface vibrational spectroscopy, high pressure scanning tunneling microscopy (HPSTM) and ambient pressure X-ray photoelectron spectroscopy (APXPS).

Program Impact:
This program benefits from the strong and synergistic collaboration of three investigators with expertise in catalysis, surface science, friction and lubrication, and synthesis of nanomaterials. The expertise of these investigators is complementary and their interests overlaps in many areas, resulting in joint experiments, sharing of students and postdocs. Gabor Somorjai focuses on surface structure, chemical bonding, reaction studies, and biomolecule adsorption on surfaces. Peidong Yang designs and synthesizes nanoparticle catalysts with control of parameters such as size, shape, and composition. He develops strategies for assembling metallic and bimetallic nanocrystals on surfaces. Miquel Salmeron focuses on surface characterization using scanning probe techniques that resolve single atoms and molecules and their dynamics in conjunction with theoretical studies using DFT and image simulations, single molecule manipulation, and reactions via excitation of vibrations and electronic transitions. He also investigates the structure of liquid thin and organic films using atomic force microscopy and electron spectroscopy to study friction and lubrication phenomena at the molecular level. Instrument development for surface and nanoparticle characterization is an important component of the research of the team to expand the application to practical situations under ambient gas pressures and temperatures with the goal of discovering new phenomena. This program is in line with the DOE grand challenges of control of matter at the single atom level, in energy conservation and efficiency by providing the scientific foundation for the development of new catalysts, and an understanding of the elementary mechanisms of energy dissipation in friction.

FY 2009 Authorized Budget (New BA): $1,460k

Program Personnel Supported in FY2009:
Principal Investigators: M. Salmeron 15%, G. Somorjai 5%
Postdoctorals: B. Choi 30%, A. Katan 20%, F. Tao 95%, P. Jiang 5%, S. Maier 50%, C. Aliaga 90%, C. Tsung 100%
Graduate Students: W. Brown 20%, D. Butcher 50%, G. Holinga 50%, C. Kliewer 40%, Y. Shi 60%, F. Martin 50%, I Stass 50%, M. Fardy 10%, B. Moshofsky 20%
Administrators: Inger Coble 90%, Theresa Short 5%, Alice Muller-Egan 10%

Interactions:
- G. Somorjai is the PI of the Project: "Synthesis, Characterization and Reactivity of Two-Dimensional Arrays of Metal Nanoparticles as Model Catalyst". Source of Support: DOE. Scope: Synthesis, characterization and reactivity of two-dimensional arrays of metal nanoparticles for strategic design of model catalysts and multipath catalytic reactions that control reaction selectivity
- G. Somorjai is the PI of the Project: "The Influence of Electron Flow at Oxide-Metal Interface on the Selectivity and Turnover Rates of Catalytic Reactions". Source of Support: DOE, Chemical Sciences. Scope of work: Fabrication of catalytic nanodiodes and mechanism of hot electron production by exothermic catalytic reactions. This is different from the current project, which focuses on the mechanism of photon generated hot electron production.
- G. Somorjai and M. Salmeron are co-PI, along with Hans Frei and Dean Toste, of the "Nanoscience and Nanoparticles for 100% Selective Catalytic Reactions". Source of Support: DOE, Chemical Science Division.

Scope of work: Synthesis, characterization and reactivity of three-dimensional high surface area nanoparticle systems to achieve 100% selective catalytic reactions

- M. Salmeron and Peidong Yang are co-PI, along with Paul Alivisatos, Jean Fréchet, and Lin Wang Wang of the NSET Project "Self-Assembly of Organic/Inorganic Nanocomposite Materials". Support from DOE Materials Science Division. Scope of work: Study of the electronic structure and electrical transport properties of semiconductor nanoclusters, nanorods and nanowires used for solar cell applications and of the organic molecules used for charge transfer between the nanostructures and with electrodes that connect them to the outside circuit.
- M. Salmeron is the Scientific Director of the Imaging of Manipulation Facility in the Molecular Foundry. Support from DOE. Scope of work: Provide user support to Molecular Foundry users in the area of atomic scale imaging. Advance the frontiers of instrumentation for atomic scale imaging.
- Peidong Yang is PI in the Project: "Nanowire based functional device and assembly". Source of Support: DOE. Scope of work: Explore the fundamental aspects of nanowire growth and assembly, with a focus on their photonic properties.
- Peidong Yang is co-PI in the Project: "Thermoelectric nanostructures". Source of Support: DOE. Scope of work: Nanoscale defect engineering to tune the phonon transport within bulk nanostructures materials in order to develop thermoelectrics with much enhanced ZT.

FWP Title: Microscopy Investigations of Nanostructured Materials **Name of the Laboratory: LBNL**
FWP Number: KC3103 **B&R Code: KC020301**

Program Abstract:
Nanostructured materials offer great potential for novel ways to generate, utilize, store and transport energy for the nation's economy. In this program a goal is the development of state-of-the-art optical characterization microscopies that provide higher spatial, spectroscopic, and time resolutions than are afforded by conventional techniques. To achieve these goals, laser sources are coupled with a variety of scanned probe and confocal microscopies to obtain high performance apertureless near field microscopy for enhancing spatial resolution, single-molecule or single-nanostructure spectroscopies for fluorescence intermittency studies, coherent anti-Stokes Raman microscopy for greatly improved spectral resolution, and ultrafast pump-white light probing for time dynamics studies. These techniques are applied to problems in semiconductor nanostructured materials, such as the measurement of carrier lifetimes, the optical identification and energy transfer between dissimilar materials of nanodots and islands, and the full spectral characterization of polymer crosslinking.

Program Impact:
Development of novel microscopies, such as coherent anti-Stokes Raman scattering (CARS) microscopy using single ultrabroad band laser pulses and phase control, as well as apertureless near field scanning optical microscopy (ANSOM), provide new spectral and spatial windows into the analysis of materials. Introduction of pump-probe ultrafast spectroscopies and fluorescence intermittency studies provide new ways to interrogate time dynamics in nanostructured materials. DOE-BES missions in energy production are addressed by this effort through the characterization of materials that can enhance the opportunity for solar energy utilization.

FY 2009 Authorized Budget (New BA): $390K

Program Personnel Supported in FY2009:

Postdoctorals: Y. Abate 70%
Graduate Students: A. Caster 10%, A. Caughey 50%, A. Cordones 30%, P. Nagel 5%
Administrators: A. Bradford 30%, K. Fowler 30%

Interactions:
Scanning Transmission X-Ray Microscope (STXM), Advanced Light Source, Lawrence Berkeley National Laboratory (M.K. Gilles)

Inorganic Nanostructures Facility, The Molecular Foundry, Lawrence Berkeley National Laboratory (D.J. Milliron and J.J. Urban)

FWP Title: Inorganic/Organic Nanocomposites **Name of the Laboratory: LBNL**
FWP Number: KC3104 **B&R Code: KC020301**

Program Abstract:
The goal of this project is to develop new methods by which we can create functional materials by parallel and hierarchical self-assembly. We seek to develop wet chemical processes by which organic/inorganic composites can be created with a high degree of control on many length scales simultaneously. By developing a comprehensive ability to pattern organic/inorganic composites, it will be possible to design complex materials in which several microscopic processes are independently and simultaneously optimized. We target functional materials with applications in energy conversion, mechanical composites, and optical/electrical devices. The team: Paul Alivisatos (Nanocrystals); Jean Frechet (Organic Components); Miquel Salmeron (Imaging) ; P. Yang (Nanowires), Lin Wang Wang (Theory); Ting Xu (block copolymers).

Program Impact:
The fundamental science of how to achieve a high level of control of matter on multiple length scales, to produce hybrids with the physical properties of inorganic components and yet the assembly flexibility of organics is a major challenge for Basic Energy Sciences. This project leverages the expertise of a diverse group of PIs with expertise in inorganic nanomaterials (Alivisatos and Yang), organic nanomaterials (Freceht and Xu) as well as theory (Lin Wang Wang) and advanced characterization (Salmeron). This team works in coordinated fashion to develop nanocomposites and to examine their functionality. Developed the concept of hybrid inorganic-organic nanorod – polymer solar cells (Science 2002, *295*, 2425) and dual nanocrystal solar cell (Science 2005). Developed a general route to vertical ZnO nanowire arrays using textured ZnO seeds and prepared nanowire dye-sensitized solar cells (Nature Materials, 2005) and core-shell nanowire dye sensitized solar cells (J. Phys. Chem. B, 2006). Demonstrated the growth of InGaN nanowires (Nature Mater., 2007). Developed the silicon nanowire radial p-n junction solar cell (JACS, 2008). Calculated the energy levels of semiconductor nanorods and nanowires, and heterostructures made from them. Demonstrated the synthesis in high yield of branched nanocrystals(Nature Materials, 2003) and hyper-branched nanocrystals (Nano Letters, 2005). Conducted electrical and AFM investigations of individual inorganic tetrapods. Developed a block-copolymer-small molecule approach to assemble nanoparticles with controlled dimension of interaction for studies of transport phenomena in nanocrystal solar cells. Explored importance of polymer functionality, morphology, regioregularity, molecular weight, and MW distribution as well as the use of FRET in inorganic organic solar cells. Demonstrated strong dependence of electrical conductivity of oligothiophene molecular assemblies on crystalline order for charge transport across molecules and measured charge hopping length scale. Explained the difference in pattern formation for Ag and Cu ion exchange in CdS nanorod by surface energy calculations; studied the atomic structures of ZnO/P3HT attachment via ab initio calculations.

FY 2009 Authorized Budget (New BA): $1,253k

Program Personnel Supported in FY2009
Principal Investigators: J. Frechet 5%
Postdoctorals: H. Zheng 50%, W. Ma 100%, C. Piliego 70%, X. Zhao 30%, B. Hendriksen 70%, A. Katan 10%
Graduate Students: S. Brittman 40%, I. Jen-LaPlante 5%, B. Wiers 5%, B. Rancatore 40%, F. Martin 5%, D. Unruh 20%, D. Kavulak 20%, T. Clem 50%, M. Sheldon 10%
Technical Staff: J. Wang 40%
Administrator: C. Ramiro 40%, R. Tidwell 40%

Interactions: 3M, Canon, Dow Chemical, Dupont, Intel, Kodak, Motorola, Xerox; Bayer, BASF, Mitsubishi Chemical, Nanosys, Solexant, Samsung. Wanli Yang, Andrew Canning, Jose Manuel Roldan, Univ. Jaen, Spain, for electronic structure calculations of their special polymer systems; Yong Zhang, Univ. North Carolina, Charlotte, charge patching model for alloy electronic structure calculations.

FWP Title: Physical Chemistry of Semiconductor Nanocrystals **Name of the Laboratory: LBNL**
FWP Number: KC3105 **B&R Code: KC020301**

Program Abstract:
Nanometer size inorganic crystals are playing an increasingly important role in solid-state physics, chemistry, materials science, and even biology. Many fundamental properties of a crystal (e.g., ionization potential, melting point, band gap, saturation magnetization) depend upon the solid being periodic over a particular length scale, typically in the nm regime. By precisely controlling the size and surface of a nanocrystal, its properties can be tuned. Using techniques of molecular assembly, new nanocrystal-based materials can in turn be created. This program encompasses fundamental studies of the mechanisms and kinetics of nanocrystal synthesis, studies of chemical transformation of nanocrystals via addition, substitution, and branching, as well as studies of scaling laws for optical, electrical, magnetic, and structural size dependent properties

Program Impact:
This program tightly integrates capabilities in nanocrystal synthesis and nanocrystal properties measurements with theoretical and computational tools, imaging tools, and characterization techniques of Berkeley Lab, in such a way as to create a comprehensive system for the development and understanding of colloidal nanocrystals. The program has had enormous impact in diverse areas of fundamental science that underpin diverse energy technologies. It helped develop the concept of inorganic nanocrystals as a class of macromolecule. First studies of surface derivitization and isolation of nanocrystals, and immobilization of nanocrystals on self-assembled monolayers; first photoelectron spectroscopy studies of nanocrystal electronic structure (with Jim Tobin) and nanocrystal surface structure. X-ray Absorption Spectroscopy as a tool for determining nanocrystal surface structure; first measurements of single nanocrystal x-ray absorption spectra. Synthesis and shape control of semiconductor nanocrystals and nanorods of CdSe, InP, InAs, GaAs, Co, and Fe_2O_3. Discovery of branching in nanorod synthesis of II-VI semiconductors, including synthesis of tetrapods and inorganic dendrimers. Studies of core-shell nanocrystal synthesis and properties. Optical properties of nanocrystals, including hole-burning, resonance Raman, photon echo, Stark effect; polarization and blinking studies of quantum dots and nanorods. Studies of pressure and temperature induced structural transformations in nanocrystals. Single nucleation events in nanocrystal structural transformations; shape change as an indicator of mechanism in nanocrystal transformations, first measurements of activation energy and activation volume in nanocrystal structural transformations. Shock wave studies of nanocrystals; Hollow nanocrystal formation through the nanoscale Kirkendall effect. Cation and anion exchange kinetics, reversibility, mechanism in nanocrystals. First electrical device based on a nanocrystal-polymer composite (light emitting diode); first transistor based on a single nanocrystal and a single molecule (with Paul McEuen); developed the use of DNA as a tool for patterning nanocrystals (with Peter Schultz); discovered liquid crystal phases of semiconductor nanorods; introduced the use of colloidal quantum dots as fluorescent biological labels (with Shimon Weiss); first demonstrated the plasmon spectroscopic ruler for measuring nanoscale distances. Hybrid nanorod-polymer solar cell. Dual Nanocrystal Solar cell. Mechanical studies of individual nanoparticles. Studies of chemical transformation of individual nanocrystals.

FY 2009 Authorized Budget (New BA): $615k

Program Personnel Supported in FY2009:
Postdoctorals: J. Owen 70%, P. Trudeau 20%, J. Beeman 5%
Graduate Students: K. Koski 15%, A. Mastroianni 5%, J. Park 20%, B. Sadtler 40%, J. Smith 20%, C. Wadia 30%, J. Wang 50%, J. Wittenberg 20%
Administrator: R. Tidwell 40%

Interactions:
Current collaborators: Jan Liphardt, Phil Geissler, Jean Frechet, Ting Xu, Delia Milliron, Jeff Urban, Uri Banin, Alex Pines, Ned Seeman, Don Tilley, Harry Atwater, Nate Lewis, Wendell Lim, Dyche Mullins, Charlie Craik; Jim Wells, Heinz Frei; Founder, Quantum Dot Corporation (now part of Life Tech Inc.); Nanosys, Inc; Solexant, Inc.

FWP Title: Nuclear Magnetic Resonance **Name of the Laboratory: LBNL**
FWP Number: KC3107 **B&R Code: KC020301**

Program Abstract:
The nuclear magnetic resonance (NMR) program has two complementary components. The first is the establishment of new concepts and techniques in NMR and its offspring, magnetic resonance imaging (MRI), in order to extend their applicability and enhance their capability to investigate molecular structure and organization from materials to organisms. The study and diagnostic use of nuclear spins interacting with each other and with others degrees of freedom requires the development of new theoretical and experimental methods; one consequence of these efforts is the design and fabrication of next-generation NMR and MRI equipment. The second component of the research program involves the application of such novel methods, together with other programs, and with outside laboratories and industry, to significant problems in chemistry, materials science, and biomedicine. It is the unique environment of interdisciplinary research and large-scale instrumentation capabilities at the Lawrence Berkeley National Laboratory that cultivates these innovations, their diverse applications, and technology transfer.

Program Impact:
"Seeing is believing" novel techniques and devices of magnetic resonance spectroscopy and imaging have expanded our ability to "see" into materials and organisms. The concepts and instrumentation, adopted worldwide by laboratories and industry, are being used to investigate molecular structure and organization from the nanoscale dimensions of catalysts and polymers to the macroscopic proportions of human imaging and oil exploration. Education: hundreds of scientists ("Pinenuts") trained in the laboratory, many of them hold leading positions in academia and industry. Patents: nearly forty issued, filed, pending or disclosed methodologies licensed, adapted into commercial NMR technology. Journal Covers and News Recognition: eg Nature, Nature Materials, Nature "News and Views", Science, Science "Perspectives", Technology Review, Photonics.com, New Scientis, Spectroscopy, J. Mag. Resonance, Angewandte Chemie, J. Physical Chemistry, C&E News, Science News, Biophotonics, Analytical Chemistry, R&D Magazine, PNAS "Commentary", Physics World, Scientific American.

FY 2009 Authorized Budget (New BA): $1,000k

Program Personnel Supported in FY2009:
Principal Investigator: A. Pines 15%
Postdoctorals: V. Bajaj 100%, L. Chen 5%, G. Kervern 80%, X. Zhou 100%, L. Schroeder 60%
Graduate Students: C. Crawford 20%, M. Donaldson 30%, P. Ganssle 30%, D. Graziani 20%, N. Halpern-Manners 10%, J. Mustonen 10%, J. Paulsen 30%, R. Ramirez 30%, D. Trease 30%
Administrator: A. Jacobson 90%

Interactions:
D. Wemmer (Physical Biosciences and Chemistry), J. Clarke (MSD and Physics), D. Budker (NSD and Physics), T. Budinger (LSD and Bioengineering), M. Francis (MSD and Chemistry). Industry: eg Schlumberger-Doll Research, Chevron, Varian, General Electric, T2 Biosystems, J.Kitching NIST.

Related Project URL: http://waugh.cchem.berkeley.edu

FWP Title: Plastic Electronics **Name of the Laboratory: LBNL**
FWP Number: KC3108 **B&R Code: KC020301**

Program Abstract:
The plastics electronics program is directed towards acquiring a fundamental understanding of the molecular and physical principles that govern the design of electroactive and responsive organic materials. Major components of the program are directed towards the fundamental design and synthesis of novel organic materials, both small molecules and polymers, the determination of their physical and electronic properties, and the exploration of approaches for application of these materials in energy related issues where organic materials can make a significant contribution through their intrinsic properties.

Program Impact:
This program directed towards a fundamental understanding of structure property relationships for electroactive materials useful in plastic electronics requires both significant materials synthesis, materials characterization, and materials physics efforts. The program has a foundation in the molecular design of electroactive molecules (Frechet) which requires extensive support in physical methods (Segalman) using for example the facilities of the Advance Light Source or the Stanford Synchrotron, as well as specialized studies in polymer physics using for example the equipment purpose built by Professor C. Harris and his group. In addition the program relies heavily on a centralized research facility for the fabrication of test devices, which enables the functional characterization of the new materials the study of the effect of morphology on performance, etc. Such a facility with the breadth of expertise required could not arise from a single investigator grant.

FY 2009 Authorized Budget (New BA): $1,000,000

Program Personnel Supported in FY2009:
Principal Investigators: J. Frechet 5%, C. Harris 10%, R. Segalman 10%
Postdoctorals: C. Piliego 20%, X. Zhao 30%, B. Boudouris 10%, Y. Hong 30%; Leveraged postdoctorals (external fellowships): Pierre Beaujuge 50%, Stefan Pastine (50%), Y. Miyamoto (100%). B.J. Kim (50%).
Graduate Students: P. Armstrong 50%, C. Mauldin 50%, D. Poulsen 50%, F. Liao 10%, S. Yin 10%, J. Johns 50%, V. Ho 5%; Leveraged graduate students (External Fellowships) C. Woo (50%), T. Holcombe (50%)
Administrators: C. Gliebe 30%, C. Ramiro 50%

Interactions:
Michael McGehee (Materials Physics) Stanford University; Michael Graetzel EPFL Switzerland; A. Zettl (Physics), Berkeley; Dean Delongchamps (Neutron Scattering, NIST); Michael Toney (Scattering studies, Stanford Synchrotron), Vivek Subramanian (Electrical Engineering, ink jet printing of devices. Berkeley).

FWP Title: Biomolecular Materials **Name of the Laboratory: LBNL**
FWP Number: KC3109 **B&R Code: KC020301**

Program Abstract:
The premise underlying The Biomolecular Materials Program is that living organisms have evolved molecules, structures, processes and approaches to achieve functions that can be used or mimicked to produce materials, devices or concepts for application in non-biological environments. This is to be distinguished from Biomaterials programs which seek to develop solutions-- such as implants, artificial organs, drug delivery systems--to biomedical problems afflicting humans and animals. Specific projects in the program include

- building and manipulating models of membranes and membrane receptors for the study of coatings and functional "hybrid structures" of living cells and non-living devices;
- design and synthesis of carbohydrates for controlled interface properties;
- design and synthesis of proteins, dendrimers and DNA oligomers for spatial patterning of inorganic nanocrystals and functional assemblies.
- Theory work supports the experimental work.

Selected examples of research targets include the

- controlled fabrication of protein/lipid/nanoparticle surfaces to study the interaction between cells and non-living surfaces;
- development of novel and selective chemical synthetic techniques to modify viral capsids so that they can be used to template the elements of complex, multi-component interacting systems such as artificial light harvesting complexes;
- advancement of techniques to specifically arrange nanocrystals in space using the base-pairing capabilities of DNA so that those nanocrystals can be used as reporters of molecular structures and molecular events of importance including, for example, the structure of DNA, the nature of important and useful chemical reactions, and optical studies of molecular events.
- fundamental exploration of synthetic macromolecules as mimics of catalytic proteins
- exploration of molecular shape and microenvironment in bio-inspired catalytic macromolecular systems

Program Impact:
Success in a program of this sort requires the close collaboration of multiple disciplines. Knowledge of Biology and Biochemistry is essential to the identification of appropriate biological targets and the understanding of their intricate and subtle structures and functions; synthetic organic chemistry is critical to the design of schemes to make the molecules and structures that mimic the naturally occurring molecules and structures; physical chemistry is required for the non-biological aspects of the devices, processes and structures, and theory work crossing the disciplines is necessary to predict structures and phenomena, direct their synthesis and explain the results. The National Laboratory structure is critical to our ability to bring senior investigators, postdocs and students from these various disciplines together. The impact of a successful program in this area is extremely broad in that billions of years of evolution have allowed Nature the opportunity to solve a wide variety of materials problems in ways that materials scientists have not before conceptualized or developed; thus this approaches opens doors to the developent of a wide variety of materials problems that were, until now, closed to us.

FY 2009 Authorized Budget (New BA): $850k

Program Personnel Supported in FY2009:
Principal Investigators: P. Geissler 10%
Postdoctorals: Y. Jun 50%, K. Godula 90%, R. Jasti 70%, V. Rodionov 60%, A. Widmer-Cooper 100%
Graduate Students: S. Sheikholeslami 50%, D. Finley 30%, S. Scroggins 30%, R. Petit 30%
Administrator: K. Carkhuff 30%

Interactions: Primary collaborations involve theory-experiment linkages, along with sharing of synthetic and characterization skills among groups specializing in proteins, carbohydrates, membranes and fundamental organic synthesis techniques.